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* * * * * * * * * * *   Welcome to STN International   * * * * * * * * * * *
* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

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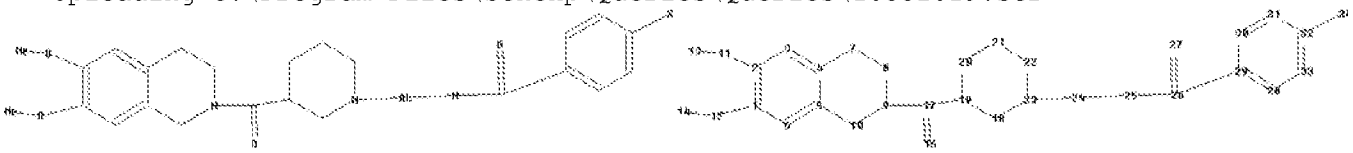

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ring nodes :
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chain bonds :
1-12  2-11  9-17  11-13  12-14  16-17  17-19  23-24  24-25  25-26  26-29  26-27
32-34
ring bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-10  7-8  8-9  9-10  18-19  18-23  19-20  20-21
21-22  22-23  28-29  28-33  29-30  30-31  31-32  32-33
exact/norm bonds :
1-12  2-11  4-7  5-10  7-8  8-9  9-10  9-17  16-17  18-19  18-23  19-20  20-21  21-
22  22-23  23-24  24-25  25-26  26-27
exact bonds :
11-13  12-14  17-19  26-29  32-34
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  28-29  28-33  29-30  30-31  31-32  32-33
isolated ring systems :
containing 1 : 18 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
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L5   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2000:881143  CAPLUS  Full-text
DN   134:42075
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TI Preparation of novel isoquinoline derivatives as If current inhibitors
IN Watanabe, Toshihiro; Kakefuda, Akio; Okazaki, Toshio; Masuda, Noriyuki; Wada, Koichi
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000075133	A1	20001214	WO 2000-JP3564	20000601 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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US 6573279	B1	20030603	US 2001-980402	20011203
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OS MARPAT 134:42075
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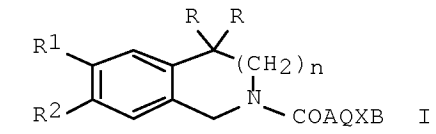

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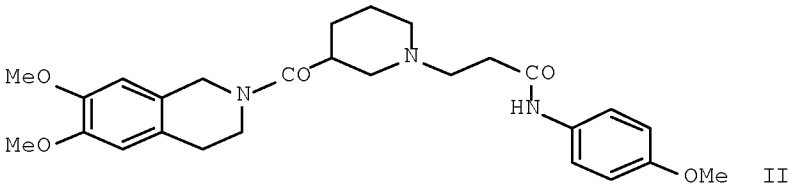

II

AB Title compds. [I; R = H, CH3; R1 = H, OCH3; R2 = H, OCH3; n = 1, 2; Q = CH2, CH2CH2, CH2CH2CH2; X = CONH, NHCO; A = pyrrolyl, pyrrolidinyl, piperidinyl; B = benzene, indenyl, pyridinyl, benzofuryl, etc.], stereoisomers, and salts having If current inhibitory effect without serious side effects such as convulsion are prepared and drugs, particularly cardiac rate lowering agents containing title compds. as active ingredient are discussed. Title compds. are useful in preventing ischemic heart diseases such as precordial anxiety (thoracic precordial anxiety) and myocardial infarct, and circulatory diseases such as congestive heart failure and arrhythmia (supraventricular arrhythmia, etc.). Thus, the title compound II was prepared

IT 312752-77-5P 312752-79-7P 312752-81-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as If current inhibitors)

RN 312752-77-5 CAPLUS

CN Benzamide, N-[2-[3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-2,4-difluoro-, ethanedioate (1:1) (CA INDEX NAME)

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CRN 312752-76-4
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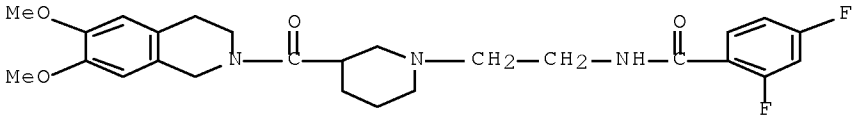

CM 2

CRN 144-62-7
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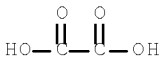

RN 312752-79-7 CAPLUS
CN Benzamide, N-[2-[3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-3-(trifluoromethyl)-, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 312752-78-6
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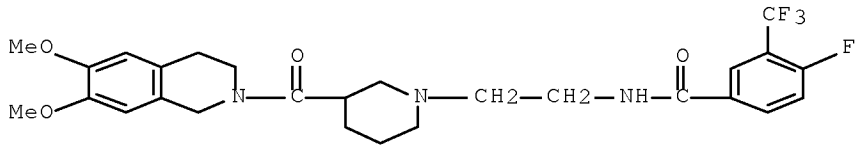

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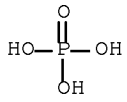

RN 312752-81-1 CAPLUS
CN Benzamide, 3-chloro-N-[2-[3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-, ethanedioate (1:1) (CA INDEX NAME)

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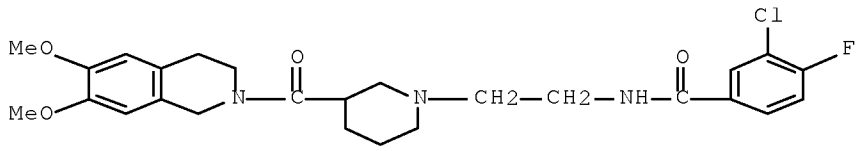

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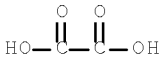

IT 312752-51-5P 312752-71-9P 312752-86-6P
312752-88-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as If current inhibitors)

RN 312752-51-5 CAPLUS

CN Benzamide, N-[2-[3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-3,4-difluoro-, ethanedioate (1:1) (CA INDEX NAME)

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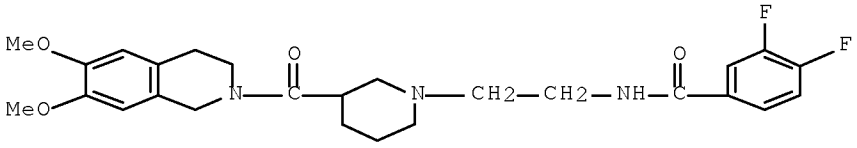

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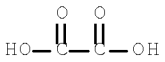

RN 312752-71-9 CAPLUS

CN Benzamide, N-[2-[3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-, ethanedioate (1:1) (CA INDEX NAME)

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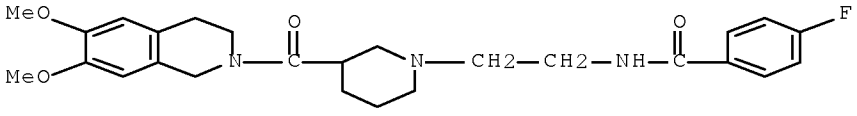

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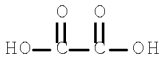

RN 312752-86-6 CAPLUS
CN Benzamide, N-[2-[(3R)-3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-, phosphate (1:1) (CA INDEX NAME)

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CRN 312752-85-5
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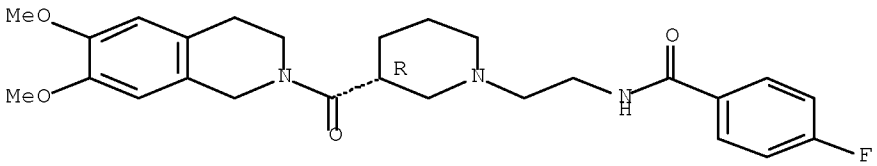
Absolute stereochemistry. Rotation (-).



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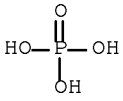
CMF H3 O4 P

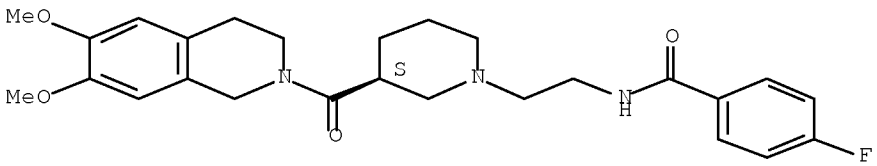


RN 312752-88-8 CAPLUS
CN Benzamide, N-[2-[(3S)-3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 312752-87-7
CMF C26 H32 F N3 O4

Absolute stereochemistry. Rotation (+).



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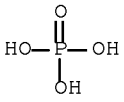

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 3 L4 NOT L5

=> dis l6 1-3 bib abs fhitstr

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:220250 CAPLUS Full-text
DN 146:221125
TI Therapeutic agent for atrial fibrillation
IN Wada, Koichi; Masuda, Noriyuki; Taniguchi, Keiichi
PA Astellas Pharma Inc., Japan
SO PCT Int. Appl., 21pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007023775	A1	20070301	WO 2006-JP316349	20060822

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CA 2617519 A1 20070301 CA 2006-2617519 20060822
EP 1917979 A1 20080507 EP 2006-796612 20060822
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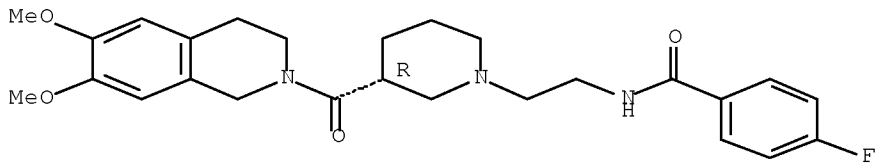
PRAI JP 2005-241403 A 20050823
WO 2006-JP316349 W 20060822

AB Disclosed is a therapeutic agent for atrial fibrillation comprising an If current inhibitor, particularly (-)-N-[2-[(R)-3-(6,7-dimethoxy-1,2,3,4-tetrahydro- isoquinoline-2-carbonyl)piperidino]ethyl]-4-fluorobenzamide monophosphate, as an active ingredient. This active ingredient has more preferred properties for use as a therapeutic agent for atrial fibrillation compared to verapamil (a Ca antagonist) and atenolol (a β-blocker) which have been conventionally used as the therapeutic agents for atrial fibrillation.

IT 312752-85-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic agents for atrial fibrillation containing If current inhibitors)

RN 312752-85-5 CAPLUS
CN Benzamide, N-[2-[(3R)-3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:872791 CAPLUS Full-text
DN 141:350046
TI Preparation of novel crystal of fluorobenzamide derivative
IN Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Yamaguchi, Sou
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004089933	A1	20041021	WO 2004-JP4794	20040401

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,

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	EP 1609788	A1	20051228	EP 2004-725182	20040401
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	IN 2005DN04378	A	20070105	IN 2005-DN4378	20050927
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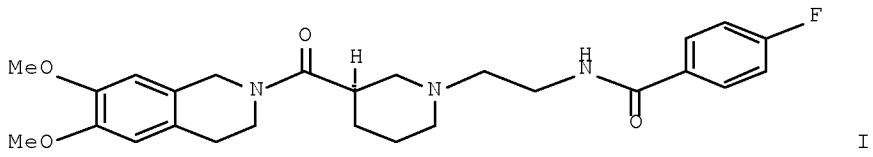


I

AB A novel crystal of (R)-(-)-N-[2-[3-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide (I) monophosphate, which is known as a preventive and/or remedy for ischemic diseases such as angina pectoris and myocardial infarction and cardiovascular diseases such as ischemic heart failure and arrhythmia, was prepared and characterized by X-ray diffraction spectra and DSC. Two crystal forms (α and β crystal forms) of compound I were prepared α Crystal form of compound I exhibited excellent moisture adsorption property and is advantageous for handling and formulation. Thus, 206.4 g (R)-1-[2-[(4-fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid was treated with 810 mL DMF and 120.8 g 6,7-dimethoxy-1,2,3,4- tetrahydroisoquinoline monohydrochloride, stirred, cooled, treated with 53.22 g Et3N at ≤12°, treated with 217 mL DMF and then successively with 21.32 g 1H-1,2,3-benzotriazole and 121.0 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride at ≤5°, and stirred at 0-4° for 15.5 h, and treated with 340 mL H2O, 2,000 mL EtOAc, and 550 mL 8% (W/V) aqueous NaOH solution to give, after workup and concentration, crude free base I (83.9% purity). I (11.90 g) was dissolved in ethanol to a total weight of 97.8 g, treated with 5 mL ethanol, 0.47 g H2O, and 0.86 g 85% H3PO4, and then with 5 mL ethanol, stirred at 30° overnight, and filtered to give, after washing the crystals with ethanol and drying, 3.38 g I monophosphate (α crystal form).

IT 312752-86-6P, (R)-(-)-N-[2-[3-[(6,7-Dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide monophosphate

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel crystal of fluorobenzamide monophosphate derivative having excellent moisture adsorption property)

RN 312752-86-6 CAPLUS

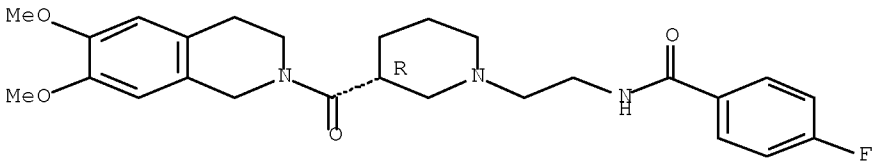
CN Benzamide, N-[2-[(3R)-3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-

isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro-, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 312752-85-5
CMF C26 H32 F N3 O4

Absolute stereochemistry. Rotation (-).



CM 2

CRN 7664-38-2
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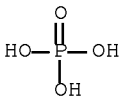

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:565208 CAPLUS Full-text
DN 141:106387
TI Isoquinoline derivatives containing benzamide moiety and process for their preparation
IN Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Kakefuda, Akio
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004058710	A1	20040715	WO 2003-JP16582	20031224

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,

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             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2511989           A1    20040715    CA 2003-2511989        20031224
     AU 2003292757        A1    20040722    AU 2003-292757         20031224
     CN 1753870           A     20060329    CN 2003-80109919       20031224
     IN 2005DN02787       A     20070105    IN 2005-DN2787         20050623
     US 20060084807       A1    20060420    US 2005-540421         20050624
     KR 758522            B1    20070914    KR 2005-711965         20050624
PRAI JP 2002-375153       A     20021225
     WO 2003-JP16582      W     20031224
OS   MARPAT 141:106387
GI
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

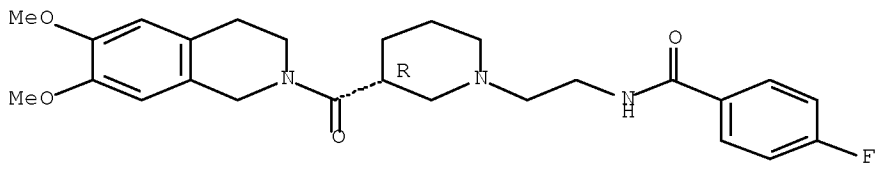
AB Process for the preparation of compds. I [R3 =, R4 = H, alkyl, alkoxy; Ar = (un)substituted aryl] and compds. II [R1 = H, alkyl, benzyl; R2 = H, protecting group of amino; Ar = (un)substituted aryl] were provided. For example, a mixture of compound (R)-II [R1 = Ethyl; R2 = H; Ar = 4-fluorophenyl] (37.94 g), e.g., prepared from (R)-piperidine-3-carboxylic acid Et ester L-tartaric acid salt in 4 steps, and 1 M aqueous NaOH (177 mL) in EtOH (100 mL) stirred at room temperature for 1 h. After treating the reaction with HCl to acidic pH, the solvent was azeotropically removed by toluene. Then, to a solution of the resulting residue in DMF (250 mL) were added 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (21.66 g), HOBt (7.97 g) and WSC hydrochloride (27.14 g) at 10 °C. The reaction was stirred at room temperature for 3 h, aqueous work-up followed by treatment with 85% phosphoric acid (13.65 g) in EtOH (500 mL) afforded claimed compound III phosphoric acid salt (44.25 g). Of note, compds. I are useful for prophylaxis and/or treatment of myocardial infarction, congestive heart failure, etc. (no data). The disclosed process employs less hazardous solvent.

IT 312752-85-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. via N-fluorobenzoylation of tetrahydroisoquinoline derivs.)

RN 312752-85-5 CAPLUS

CN Benzamide, N-[2-[(3R)-3-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)carbonyl]-1-piperidinyl]ethyl]-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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